Molecules in Stellar Photospheres

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Absorption lines from molecular species dominate the spectra of all cool stars, whether they are high luminosity giants and supergiants or faint dwarfs of the lower main sequence. The density and strength of the molecular transitions are so great that their presence profoundly affects the structure of the outermost stellar layers, the stellar photospheres. Because the cool stars are so important in a variety of astrophysical contexts, a program aimed at accurately modeling their photospheres and emergent spectra is being conducted.

A key component of this effort is the development and maintenance of complete molecular line tabulations. These tabulations contain all the line parameters required for computing the strength and broadening of each individual molecular line. In the past year the database has been expanded to include the isotopic line lists developed by Uffe Jorgensen of the Niels Bohr Institute for the CN A-X system, the TiO α, β, γ, γ', ε, δ, and ϕ systems, and the CH vibration-rotation, A-X, B-X, and C-X systems. The tabulations for OH and SiO vibrational-rotational lines based on newly available information have also been upgraded. This molecular line database now contains all the important isotopic lines for the following transitions:

Molecule	Transition	Number of lines
OH	Vibration-rotation	58,000
C_2	b-a	79,000
SiO	Vibration-rotation	93,000
CO	Vibration-rotation	135,000
CH	Vibration-rotation, A-X, B-X, C-X	115,000
CN	A-X	2,200,000
TiO	Vibration-rotation, A-X, B-X, C-X, E-X, b-a, c-a, b-d	12,000,000
H_2O	Vibration-rotation	308,000,000

In FY97, the database has been used in the study of the infrared spectrum of sunspots. This investigation has provided a valuable check on the accuracy of the molecular line parameters in the database. The spectra of cool stars provide relatively poor tests of molecular parameters simply because their temperatures, gravities, and, particularly, compositions are not known with much accuracy. Since accurate sunspot models are available and the solar abundances are well studied, high-resolution sunspot spectra are an excellent standard for comparison. Observed sunspot spectra have been systematically compared with theoretical spectra computed using the molecular line database. In addition to evaluating the accuracy of the massive H_2O line list developed at Ames Research Center, the line parameters for CO, SiO, and OH have been checked. Comparison of theoretical and observed sunspot spectra reveals significant discrepancies in the strengths and positions of many OH transitions. This result strongly suggests the need for additional laboratory and theoretical work on the energy-level structure and dipole-moment function of this important molecular species.

The molecular database has also been used to generate spectra for several cool stars: Alpha Boo, Alpha Tau, and RX Boo. In the case of the red giant Alpha Tau, an important infrared flux standard, observed and theoretical fluxes are being compared over more than three decades of wavelength, from 1 micron to beyond 1 millimeter. Although still in its early stages, the comparison of millimeter fluxes suggests significant modifications to accepted models of Alpha Tau.

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